

chain nodes :

7 8 9 17 18 19 20 21

ring nodes :

1 2 3 4 5 6 10 11 12 13 14 15

chain bonds :

2-17 5-7 7-8 7-9 9-11 17-18 17-20 18-19 20-21

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15

exact/norm bonds :

1-2 1-6 2-3 2-17 3-4 4-5 5-6 5-7 7-8 7-9 9-11 10-11 10-15
11-12 12-13 13-14 14-15 18-19 20-21

exact bonds :

17-18 17-20

isolated ring systems :

containing 1 : 10 :

G1:O,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 17:CLASS 18:CLASS
19:Atom 20:CLASS 21:Atom

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*
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*

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=>
Uploading structure

L1 STRUCTURE UPLOADED

=> s 11
SAMPLE SEARCH INITIATED 11:19:04 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 135 TO ITERATE

100.0% PROCESSED 135 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
PROJECTED ITERATIONS: 2003 TO 3397
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s 11 sss full
FULL SEARCH INITIATED 11:20:21 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2484 TO ITERATE

100.0% PROCESSED 2484 ITERATIONS 31 ANSWERS
SEARCH TIME: 00.00.01

L3 31 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
 ENTRY SESSION
FULL ESTIMATED COST 166.92 167.13

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=> s 13
L4 1 L3

=> d 14 bib abs hitstr

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN

Full Text

AN 2004:453187 CAPLUS

DN 141:7141

TI A preparation of piperazine derivatives, useful as 17 β -hydroxysteroid dehydrogenase type 3 inhibitors

IN Paruch, Kamil; Guzi, Timothy J.

PA Schering Corporation, USA

SO PCT Int. Appl., 49 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---|------|----------|-----------------|----------|
| PI | WO 2004046111 | A1 | 20040603 | WO 2003-US36203 | 20031114 |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NI, NO, NZ, PG, PH, PL, PT, RO, RU, SC, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UZ, VC, VN, YU, ZA, ZM | | | | |
| | RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| | CA 2506290 | AA | 20040603 | CA 2003-2506290 | 20031114 |
| | US 2004127503 | A1 | 20040701 | US 2003-713828 | 20031114 |
| | EP 1562901 | A1 | 20050817 | EP 2003-783382 | 20031114 |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| PRAI | US 2002-427263P | P | 20021118 | | |
| | WO 2003-US36203 | W | 20031114 | | |
| OS | MARPAT 141:7141 | | | | |
| GI | | | | | |

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to a prepn. of piperazine derivs. of formula I [wherein: X is CH or N; Z is O or NH, N-alkyl, or N-aryl, etc.; R1 and R2 are independently selected from (un)substituted (hetero)aryl, (hetero)arylkyl; R3 is H, OH, alkoxy, aryloxy, etc.; R4 is H, (cyclo)alkyl, (hetero)aryl, etc.; R5 is C(O)R6 or SO2R6; R6 is alkyl,

(hetero)aryl, (hetero)arylalkyl, (un)substituted amine], useful as inhibitors of type 3 17 β -hydroxysteroid dehydrogenase. The invention compds. are claimed to be useful for the treatment, prevention, inhibition, or amelioration of diseases such as prostate cancer, acne, and androgenic alopecia, etc. The invention compds. exhibited a range of 17 β -hydroxysteroid dehydrogenase type 3 binding activity from about 0.005 nM to 10 nM. For instance, piperazine deriv. II was prep'd. via amination of phenyl(trifluoromethylphenyl)methanol by (S)-2-tert-butylpiperazine (example 7) and subsequent reaction of the obtained piperazine deriv. III and piperidine deriv. IV (example 15).

IT 696644-18-5P 696644-21-0P 696644-24-3P

696644-28-7P 696644-32-3P 696644-36-7P

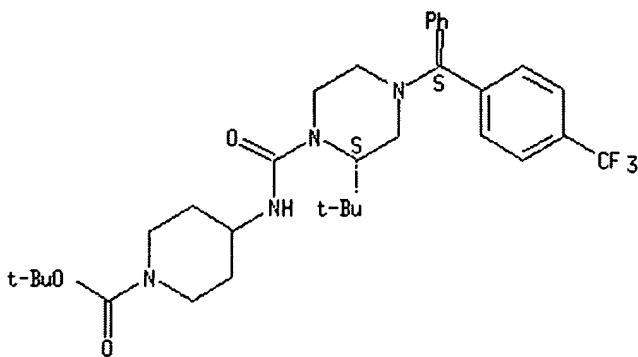
RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 17 β -hydroxysteroid dehydrogenase type 3 inhibitors for the treatment of androgen-dependent diseases)

RN 696644-18-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[(S)-phenyl[4-(trifluoromethyl)phenyl]methyl]-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

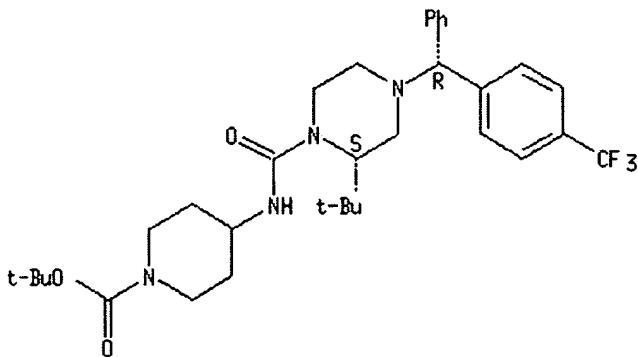
Absolute stereochemistry.



RN 696644-21-0 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[(R)-phenyl[4-(trifluoromethyl)phenyl]methyl]-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

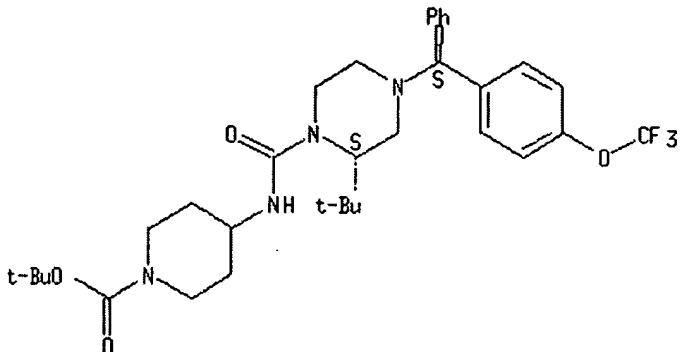
Absolute stereochemistry.



RN 696644-24-3 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[(S)-phenyl[4-(trifluoromethoxy)phenyl]methyl]-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

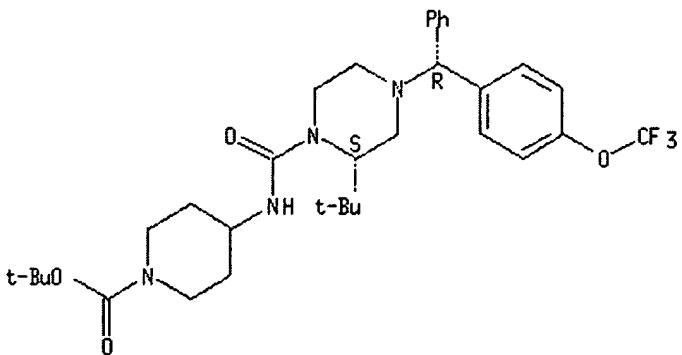
Absolute stereochemistry.



RN 696644-28-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[(R)-phenyl[4-(trifluoromethoxy)phenyl]methyl]-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

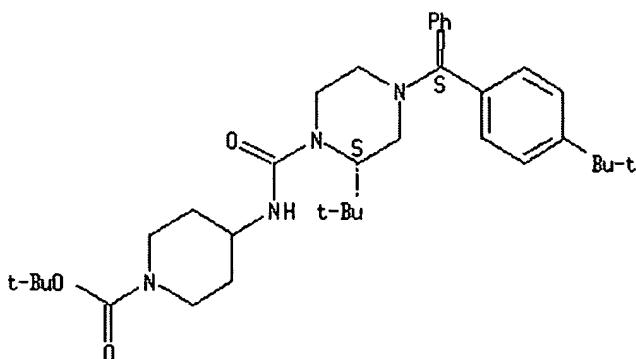
Absolute stereochemistry.



RN 696644-32-3 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[(S)-[4-(1,1-dimethylethyl)phenyl]phenylmethyl]-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

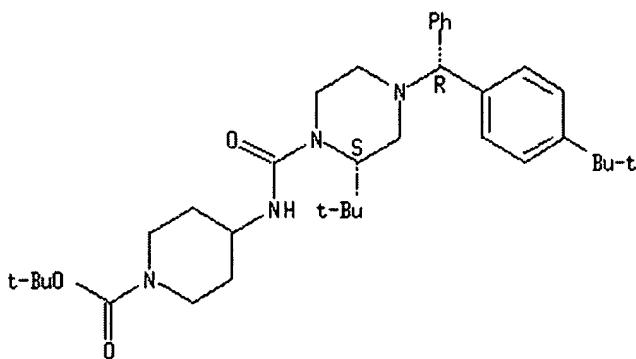
Absolute stereochemistry.



RN 696644-36-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[(R)-[4-(1,1-dimethylethyl)phenyl]phenylmethyl]-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 696643-77-3P 696643-81-9P 696643-85-3P

696643-88-6P 696643-92-2P 696643-96-6P

696644-00-5P 696644-12-9P 696644-15-2P

696644-40-3P 696644-45-8P 696644-50-5P

696644-54-9P 696644-58-3P 696644-60-7P

696644-64-1P 696644-66-3P 696644-68-5P

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696644-99-2P

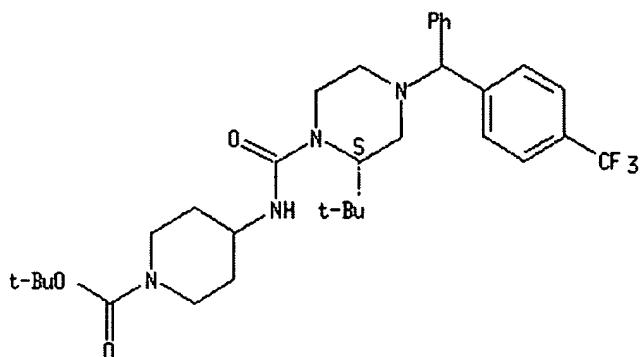
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 17 β -hydroxysteroid dehydrogenase type 3 inhibitors for the treatment of androgen-dependent diseases)

RN 696643-77-3 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[phenyl[4-(trifluoromethyl)phenyl]methyl]-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

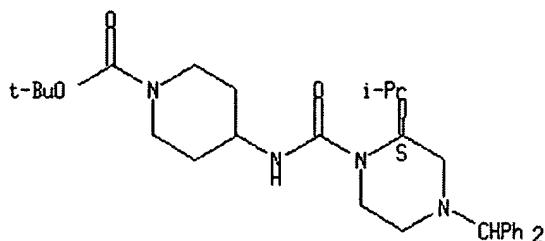
Absolute stereochemistry.



RN 696643-81-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-4-(diphenylmethyl)-2-(1-methylethyl)-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI)
(CA INDEX NAME)

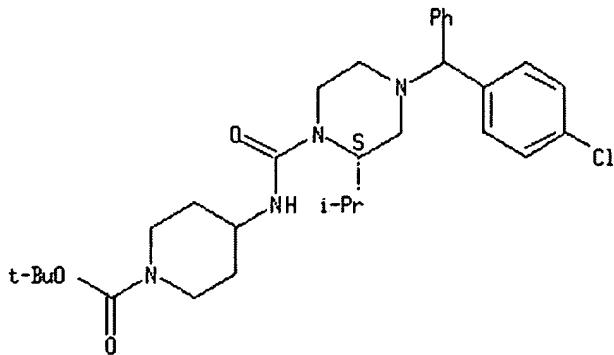
Absolute stereochemistry.



RN 696643-85-3 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-4-[(4-chlorophenyl)phenylmethyl]-2-(1-methylethyl)-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

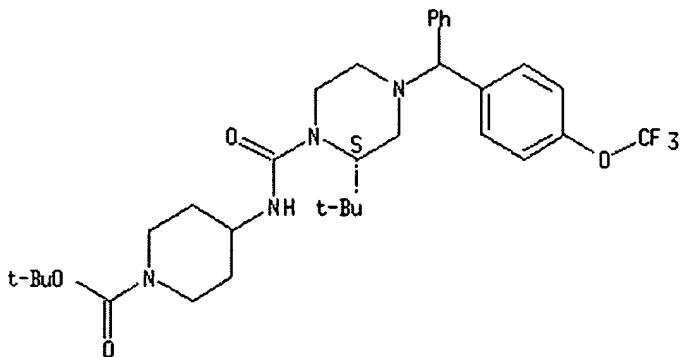
Absolute stereochemistry.



RN 696643-88-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[phenyl[4-(trifluoromethoxy)phenyl]methyl]-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

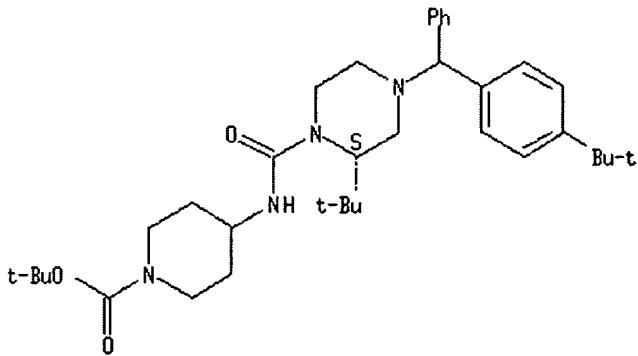
Absolute stereochemistry.



RN 696643-92-2 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[(4-(1,1-dimethylethyl)phenyl]phenylmethyl]-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

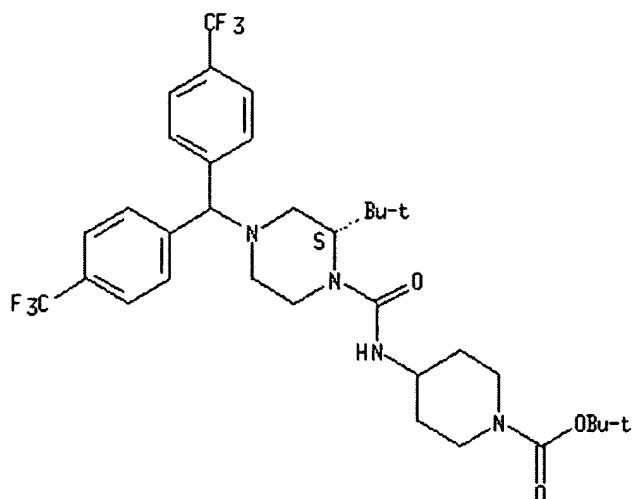
Absolute stereochemistry.



RN 696643-96-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-4-[bis[4-(trifluoromethyl)phenyl]methyl]-2-(1,1-dimethylethyl)-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

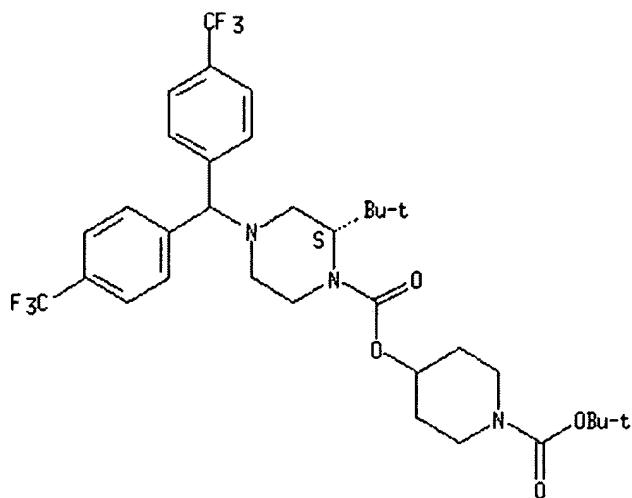
Absolute stereochemistry.



RN 696644-00-5 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[bis[4-(trifluoromethyl)phenyl]methyl]-2-(1,1-dimethylethyl)-, 1-[(1,1-dimethylethoxy)carbonyl]-4-piperidinyl ester, (2S)- (9CI) (CA INDEX NAME)

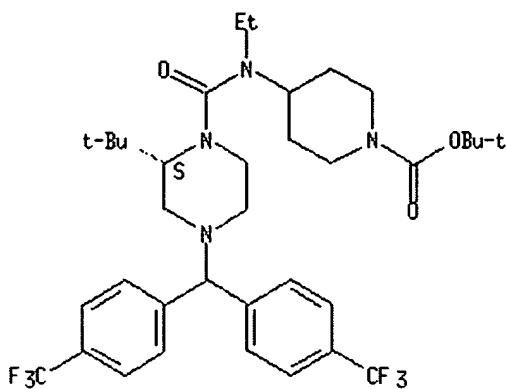
Absolute stereochemistry.



RN 696644-12-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-4-[bis[4-(trifluoromethyl)phenyl]methyl]-2-(1,1-dimethylethyl)-1-piperazinyl]carbonyl]ethylamino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

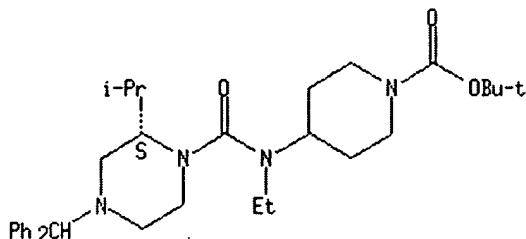
Absolute stereochemistry.



RN 696644-15-2 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-4-(diphenylmethyl)-2-(1-methylethyl)-1-piperazinyl]carbonyl]ethylamino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

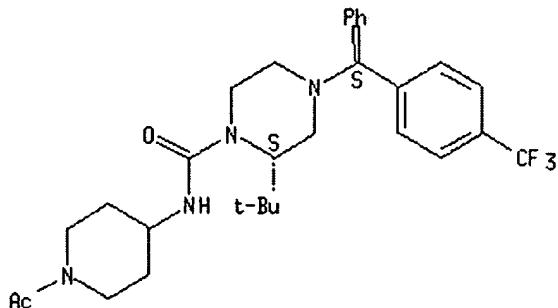
Absolute stereochemistry.



RN 696644-40-3 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-2-(1,1-dimethylethyl)-4-[(S)-phenyl[4-(trifluoromethyl)phenyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

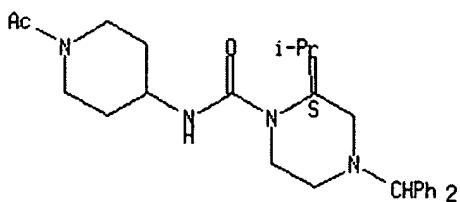
Absolute stereochemistry.



RN 696644-45-8 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-4-(diphenylmethyl)-2-(1-methylethyl)-, (2S)- (9CI) (CA INDEX NAME)

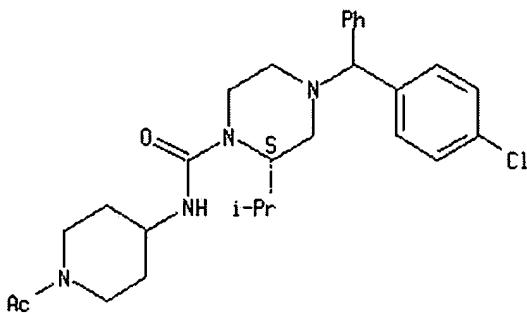
Absolute stereochemistry.



RN 696644-50-5 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-4-[(4-chlorophenyl)phenylmethyl]-2-(1-methylethyl)-, (2S)- (9CI) (CA INDEX NAME)

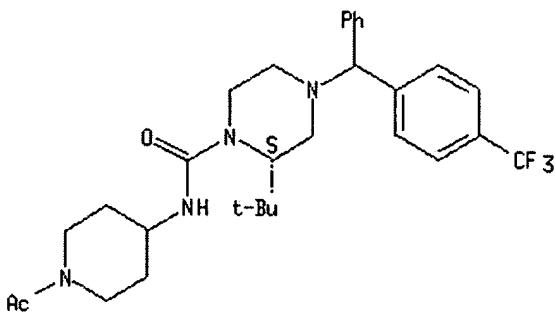
Absolute stereochemistry.



RN 696644-54-9 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-2-(1,1-dimethylethyl)-4-[phenyl[4-(trifluoromethyl)phenyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

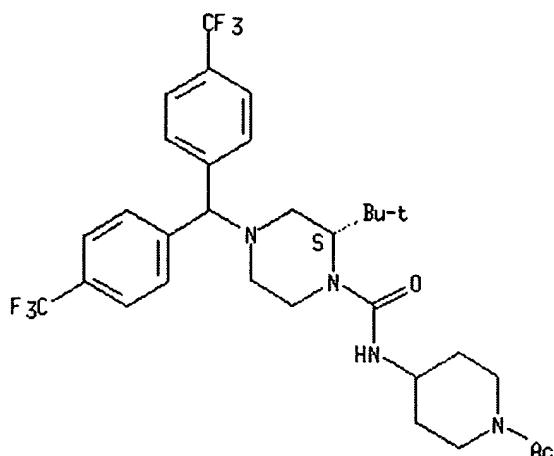
Absolute stereochemistry.



RN 696644-58-3 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-4-[bis[4-(trifluoromethyl)phenyl]methyl]-2-(1,1-dimethylethyl)-, (2S)- (9CI) (CA INDEX NAME)

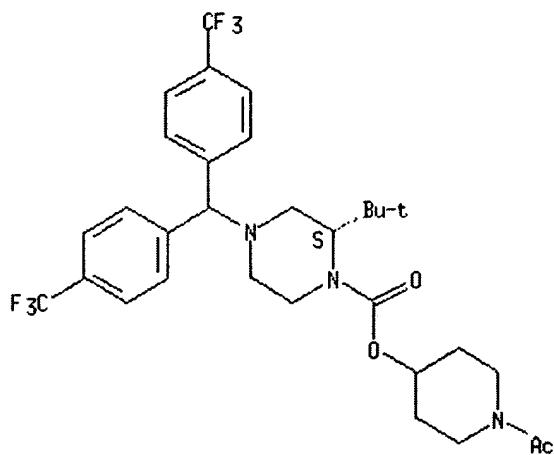
Absolute stereochemistry.



RN 696644-60-7 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[bis[4-(trifluoromethyl)phenyl]methyl]-2-(1,1-dimethylethyl)-, 1-acetyl-4-piperidinyl ester, (2S)- (9CI) (CA INDEX NAME)

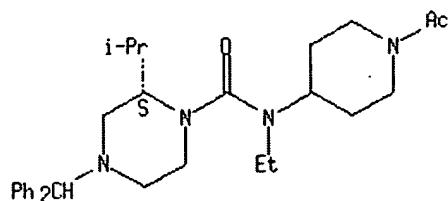
Absolute stereochemistry.



RN 696644-64-1 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-4-(diphenylmethyl)-N-ethyl-2-(1-methylethyl)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

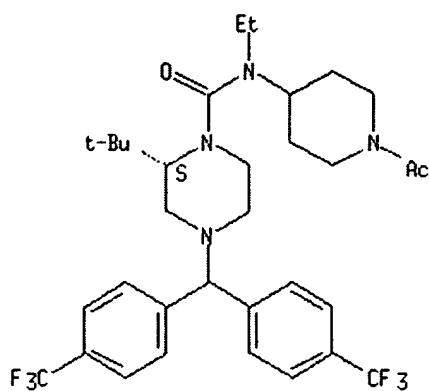


RN 696644-66-3 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-4-[bis[4-(trifluoromethyl)phenyl]methyl]-2-(1,1-dimethylethyl)-N-ethyl-, (2S)-

(9CI) (CA INDEX NAME)

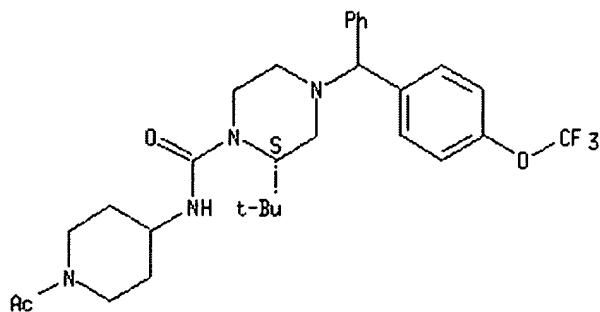
Absolute stereochemistry.



RN 696644-68-5 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-2-(1,1-dimethylethyl)-4-[phenyl[4-(trifluoromethoxy)phenyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

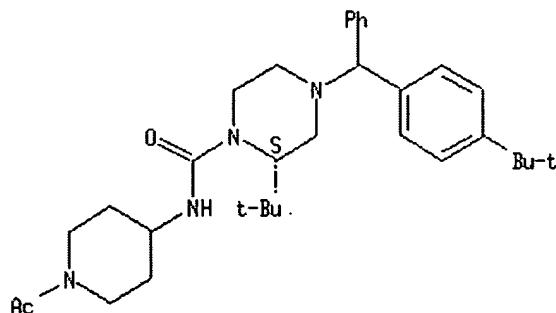
Absolute stereochemistry.



RN 696644-70-9 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-2-(1,1-dimethylethyl)-4-[(4-(1,1-dimethylethyl)phenyl)phenylmethyl]-, (2S)- (9CI) (CA INDEX NAME)

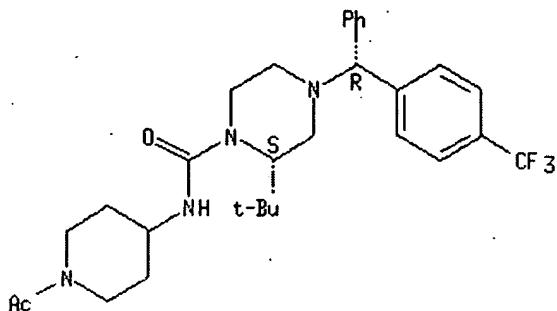
Absolute stereochemistry.



RN 696644-72-1 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-2-(1,1-dimethylethyl)-4-[*(R*)-phenyl[4-(trifluoromethyl)phenyl]methyl]-, (*2S*)- (9CI) (CA INDEX NAME)

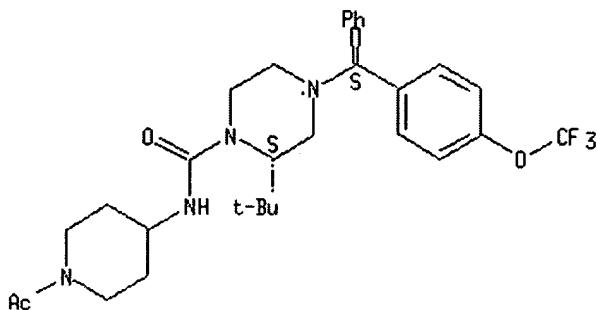
Absolute stereochemistry.



RN 696644-78-7 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-2-(1,1-dimethylethyl)-4-[*(S*)-phenyl[4-(trifluoromethoxy)phenyl]methyl]-, (*2S*)- (9CI) (CA INDEX NAME)

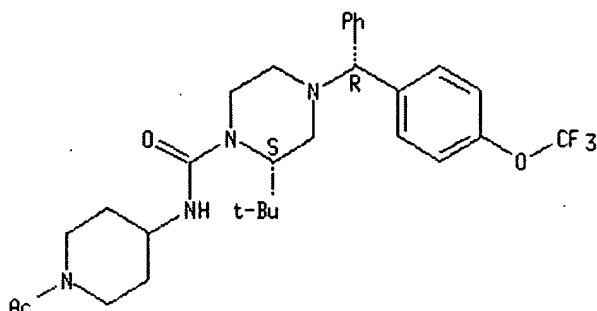
Absolute stereochemistry.



RN 696644-82-3 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-2-(1,1-dimethylethyl)-4-[*(R*)-phenyl[4-(trifluoromethoxy)phenyl]methyl]-, (*2S*)- (9CI) (CA INDEX NAME)

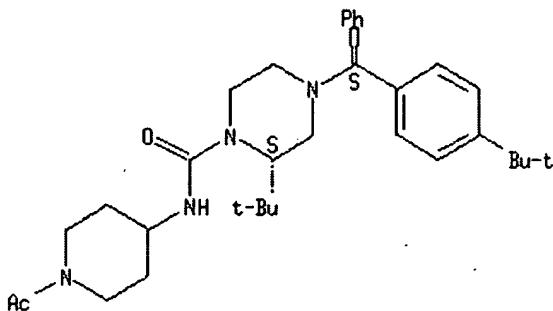
Absolute stereochemistry.



RN 696644-87-8 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-2-(1,1-dimethylethyl)-4-[(S)-[4-(1,1-dimethylethyl)phenyl]phenylmethyl]-, (2S)- (9CI) (CA INDEX NAME)

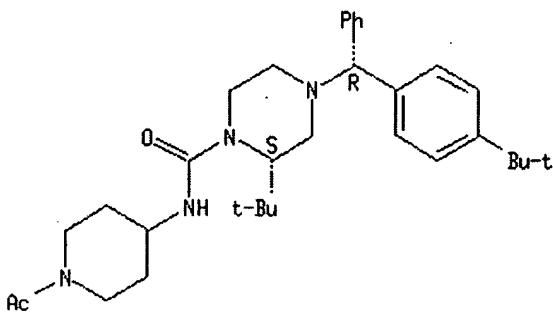
Absolute stereochemistry.



RN 696644-92-5 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-2-(1,1-dimethylethyl)-4-[(R)-[4-(1,1-dimethylethyl)phenyl]phenylmethyl]-, (2S)- (9CI) (CA INDEX NAME)

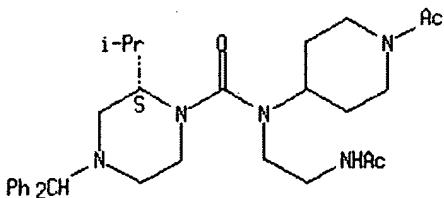
Absolute stereochemistry.



RN 696644-99-2 CAPLUS

CN 1-Piperazinecarboxamide, N-[2-(acetylamino)ethyl]-N-(1-acetyl-4-piperidinyl)-4-(diphenylmethyl)-2-(1-methylethyl)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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